Amendments to the Specification

Please replace the paragraph beginning at page 6, line 20, with the following amended paragraph.

In another aspect, the present invention provides a computer-assisted method for homology modeling an *S. aureus* peptide deformylase homolog including: aligning the amino acid sequence of an *S. aureus* peptide deformylase homolog with the amino acid sequence of *S. aureus* peptide deformylase SEQ ID NO:12 ~~SEQ ID NO:1~~ and incorporating the sequence of the *S. aureus* peptide deformylase homolog into a model of *S. aureus* peptide deformylase derived from structure coordinates set forth in Table 1 to yield a preliminary model of the *S. aureus* peptide deformylase homolog; subjecting the preliminary model to energy minimization to yield an energy minimized model; remodeling regions of the energy minimized model where stereochemistry restraints are violated to yield a final model of the *S. aureus* peptide deformylase homolog.

Please replace the paragraph beginning at page 12, line 14, with the following amended paragraph.

Figure 6 is a depiction of the secondary structure of *S. aureus* peptide deformylase. The α-helices are starred and the β-sheets are not starred. ~~Random coil connections are light gray.~~ The single Zn/Fe atom is labeled **.

Please replace the paragraph beginning at page 13, line 3, with the following amended paragraph.

Figure 12 is a stereo pair view of the superimposed alpha carbons from *S. aureus* pdf ~~(dark)~~ and *E. coli* pdf ~~(light)~~. The metal ion is indicated by the sphere.

Please replace the paragraph beginning at page 13, line 7, with the following amended paragraph.

Figure 14 a) is a schematic illustration of PCLNA inhibitor (Hao et al., *Biochemistry*, 38:

4712-19 (1999)) placing subsituents into three pdf subsites. The *S. aureus* residue number is given first with the equivalent *E. coli* amino acid subsequent. The metal ion is the labeled sphere. Figure 14 b) is a view of a surface rendering for the PCLNA complex with the E. coli enzyme with the location of the subsites indicated. ~~The light gray surface represents hydrophobic surface associated with carbon atoms, dark gray for nitrogen atoms and medium gray for oxygen atoms.~~

Please replace the paragraph beginning at page 13, line 15, with the following amended paragraph.

Figure 15 is a view of a model of the active site cleft of *S. aureus* pdf with PCLNA (from Hao et al., *Biochemistry*, 38: 4712-19 (1999)). ~~The surface is colored according to atom type with all carbons in light gray, oxygens in medium gray, and nitrogens in dark gray.~~ The six active site residues which are conserved between *E. coli* and *S. aureus* pdf are indicated ~~in white~~. These residues line the bottom of the active site.

Please replace the paragraph beginning at page 13, line 21, with the following amended paragraph.

Figure 16 is a view of a model of the surface rendering for PCLNA complex with *E. coli* enzyme (left) and of PCLNA with *S. aureus* enzyme (right). ~~The light gray colors indicate the hydrophobic surface associated with carbon atoms, dark gray is for nitrogen atoms, and medium gray for oxygen atoms.~~ Amino acid labeling indicates the surface corresponding to various residues.

Please replace the paragraph beginning at page 13, line 26, with the following amended paragraph.

Figure 17 is a stereo view of the S1 subsite of pdf with PCLNA inhibitor. The amino acid sidechains which surround the P1, caproyl group, are indicated. Labels indicate the *S.aureus* amino acid first and the equivalent *E.coli* residue second. ~~However, R97/N is indicated with the opposite nomenclature.~~

Please replace the paragraph beginning at page 35, line 21, with the following amended paragraph.

The structure coordinates set forth in Table 1 can be used to aid in obtaining structural information about another crystallized molecule or molecular complex. A "molecular complex" means a protein in covalent or non-covalent association with a chemical entity or compound. The method of the invention allows determination of at least a portion of the three-dimensional structure of molecules or molecular complexes which contain one or more structural features that are similar to structural features of *S. aureus* pdf. These molecules are referred to herein as "structurally homologous" to *S. aureus* pdf. Similar structural features can include, for example, regions of amino acid identity, conserved active site or binding site motifs, and similarly arranged secondary structural elements (e.g., α helices and β sheets). Optionally, structural homology is determined by aligning the residues of the two amino acid sequences to optimize the number of identical amino acids along the lengths of their sequences; gaps in either or both sequences are permitted in making the alignment in order to optimize the number of identical amino acids, although the amino acids in each sequence must nonetheless remain in their proper order. Preferably, two amino acid sequences are compared using the Blastp program, version 2.0.9, of the BLAST 2 search algorithm, as described by Tatusova et al., *FEMS Microbiol Lett.*, 174:247-50 (1999), and available on the world wide web at [[http://www.]]ncbi.nlm.nih.gov/gorf/bl2.html. Preferably, the default values for all BLAST 2 search parameters are used, including matrix = BLOSUM62; open gap penalty = 11, extension gap penalty = 1, gap x_dropoff = 50, expect = 10, wordsize = 3, and filter on. In the comparison of two amino acid sequences using the BLAST search algorithm, structural similarity is referred to as "identity." Preferably, a structurally homologous molecule is a protein that has an amino acid sequence sharing at least 65% identity with the amino acid sequence of *S. aureus* pdf (SEQ ID NO:12 ~~SEQ ID NO: 1~~). More preferably, a protein that is structurally homologous to *S. aureus* pdf includes at least one contiguous stretch of at least 50 amino acids that shares at least 80% amino acid sequence identity with the analogous portion of *S. aureus* pdf. Methods for

generating structural information about the structurally homologous molecule or molecular complex are well-known and include, for example, molecular replacement techniques.

Please replace the paragraph beginning at page 48, line 24, with the following amended paragraph.

The plasmid containing the pdf insert was purified and used to transform a competent strain of *E. coli* JM109. This cDNA clone used for protein expression and purification (R127K H185Q ~~H186Q~~, highlighted in Figure 3) contained two mutations. The second mutation is confirmed to be in the HIS6 tag (near the c-terminus) and has no effect on Km or Kcat. The gene encodes a total of 189 residues including a c-terminal hexahis tag (SEQ ID NO:12).